

Nadolol tri-TMS derivative

Other names:	Nadolol, O,O',O''-tris(trimethylsilyl)- Nadolol, tris-O-TMS Nadolol tris-TMS Nadolol, tris(trimethylsilyl) ether Nadolol, 3tms derivative
Inchi:	InChI=1S/C26H51NO4Si3/c1-26(2,3)27-18-21(29-32(4,5)6)19-28-23-15-13-14-20-16-24
InchiKey:	JHQUYWHNGQKRAA-UHFFFAOYSA-N
Formula:	C26H51NO4Si3
SMILES:	CC(C)(C)NCC(COC1CCCC2C1CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C2)O[Si](C)(C)C
Mol. weight [g/mol]:	525.94
CAS:	82272-01-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	6.212		Crippen Method
rinsol	2468.00		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82272013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

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<https://www.cheméo.com/cid/119-859-7/Nadolol-tri-TMS-derivative.pdf>

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